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14. ABSTRACT
This brief report presents the progress made in the September 2004 – August 2005 period. This is primarily joint work with Ms. Aarti Sawant, graduate student working with the PI (but not supported by this project). The analysis of metal plasticity based on a (physically) rigorous connection to its origins in the mechanics of defects in elastic solids is a complex matter. The primary source of complexity arises in achieving an adequate theory that can describe the dynamics of crystal defects, namely dislocation distributions, as it arises from the interaction of the stress fields of these defects as well as applied loads. Also, simply calculating the stress field of a dislocation distribution in a body undergoing finite deformations and whose crystal elastic response is non-convex is not a trivial matter. Moreover, even if such a theory could be developed, its physical resolution would have to be in the nanometer scale, whereas the effects of the physical mechanisms described above are manifest in plasticity even at the micron scale and above, one important example being the analysis of plasticity of superalloy materials.

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NiAl superalloy modeling based on combined dislocation mechanics and phenomenological plasticity

Report 2005 and Final report for project

Amit Acharya, Carnegie Mellon University

Scope of Work

The scope of this project is a preliminary exploration of the capabilities of a recently developed theory of dislocation mechanics developed by the PI, in the context of modeling the mechanical response of NiAl superalloy material. The objective will be to look at idealized small problems involving the superalloy, and try to evaluate the capability of the theory in predicting qualitative trends related to internal stress effects on initial yield.

Progress Report

This brief report presents the progress made in the September 2004 – August 2005 period. This is primarily joint work with Ms. Aarti Sawant, graduate student working with the PI (but not supported by this project).

The analysis of metal plasticity based on a (physically) rigorous connection to its origins in the mechanics of defects in elastic solids is a complex matter. The primary source of complexity arises in achieving an adequate theory that can describe the dynamics of crystal defects, namely dislocation distributions, as it arises from the interaction of the stress fields of these defects as well as applied loads. Also, simply calculating the stress field of a dislocation distribution in a body undergoing finite deformations and whose crystal elastic response is non-convex is not a trivial matter. Moreover, even if such a theory could be developed, its physical resolution would have to be in the nanometer scale, whereas the effects of the physical mechanisms described above are manifest in plasticity even at the micron scale and above, one important example being the analysis of plasticity of superalloy materials. Consequently, a coarse-graining technique for nonlinear evolutionary system becomes essential, once a fine-scale theory of plasticity/dislocation mechanics has been constructed.

In the 2003 research summary for this project, we reported on the development of a computational model for a dislocation mechanics based theory of plasticity building on earlier work (Acharya, 2001, 2003, 2004a; Roy & Acharya, 2004). This model has been shown to make good predictions of

1. size effect
2. development of microstructure from homogeneous initial conditions under boundary conditions for homogeneous deformation in the conventional theory
3. development of a strong Bauschinger effect.

Despite the successes mentioned above, we wish to do better in plasticity modeling by avoiding phenomenology so that macroscopic response of nonlinear heterogeneous media (e.g. NiAl macroscopic response) can be probed from a fundamental point of view.

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In this connection, we are developing a coarse-graining scheme for ODE systems that views multiscale mechanics as an application of exploring dynamics on locally invariant manifolds of dynamical systems (Acharya, 2004b). We use a method of reduction involving converting the underlying autonomous ODE 'fine' system to a system of first-order, time-independent, quasilinear PDE as part of the modeling step. The latter essentially represents (local) invariant manifolds in fine phase space and the PDE system needs to be solved only once to obtain a closed, reduced system of ODE that can be exercised at run-time.

An important physical consequence of the procedure is that the coarse (reduced) model in the case of a drastic reduction in the number of variables is, more often than not, ***history-dependent***, i.e. produces self-intersecting trajectories in phase space; however, this history dependence is completely described by our method. Depending upon how energy in the coarse theory is defined, these ideas also demonstrate *non-conservative coarse behavior arising from conservative fine systems.*

We have devised an algorithm based on the above idea that works reasonably on model problems. Its effectiveness in model reduction for the Lorenz system (chaotic behavior) as well as a nonlinear Hamiltonian system has been demonstrated (Sawant & Acharya, 2004). We have also aggressively moved beyond the work just referred in developing robust computational techniques for calculating the locally invariant manifolds required for the procedure and applying it to progressively more realistic systems.

In this reporting period, we have extended the coarse-graining scheme to include the development of reduced models for functions of time-averages of the microscopic degrees of freedom and applied to difficult nonlinear model problems involving gradient flows of 'wiggly energies' and the macroscopic response of atomic chains. The details of this work has been written up in the paper Acharya & Sawant (2005) and the connection of the coarse-graining ideas in their totality to the modeling of plasticity has been described in the invited Scripta Materialia Viewpoint set article Acharya et al. (2005).

With these advances, we believe that substantial progress towards the goal of developing an adequate model for the study of plasticity in superalloy material has been made along with the development of a robust computational technique for model reduction of strongly nonlinear time-dependent systems that works without regard to an intrinsic separation of scales being present in the problem.

References

Acharya, A. (2001) A model of crystal plasticity based on the theory of continuously distributed dislocations. *Journal of the Mechanics and Physics of Solids,* **49**, 761-785.

Acharya, A. (2003) Driving forces and boundary conditions in continuum dislocation mechanics. *Proceedings of the Royal Society, A,* **459**, 1343-1363.

Acharya, A. (2004a) Constitutive analysis of finite deformation field dislocation mechanics. *Journal of the Mechanics and Physics of Solids,* **52**, 301-316.

Acharya, A. (2004b) Parametrized invariant manifolds: A recipe for multiscale modeling? *Computer Methods in Applied Mechanics and Engineering*, **194**, 3067-3089.

Acharya, A. and Sawant, A. On a computational approach for the approximate dynamics of averaged variables in nonlinear ODE systems: toward the derivation of constitutive laws of the rate type. Submitted (2005) (http://www.arxiv.org/abs/math.NA/0508627)

Acharya, A., Roy, A., and Sawant, A. Continuum theory and methods for coarse-grained, mesoscopic plasticity. Invited Scripta Materialia Viewpoint Set on 'Statistical mechanics and coarse-graining of dislocation behavior in plasticity'.

Roy, A. and Acharya, A. (2004) Finite element approximation of field dislocation mechanics, In Press, *Journal of the Mechanics and Physics of Solids*.

Sawant, A., and Acharya, A. Model reduction via parametrized invariant manifolds. Submitted. (2004) (http://www.arxiv.org/abs/math-ph/0412022).